

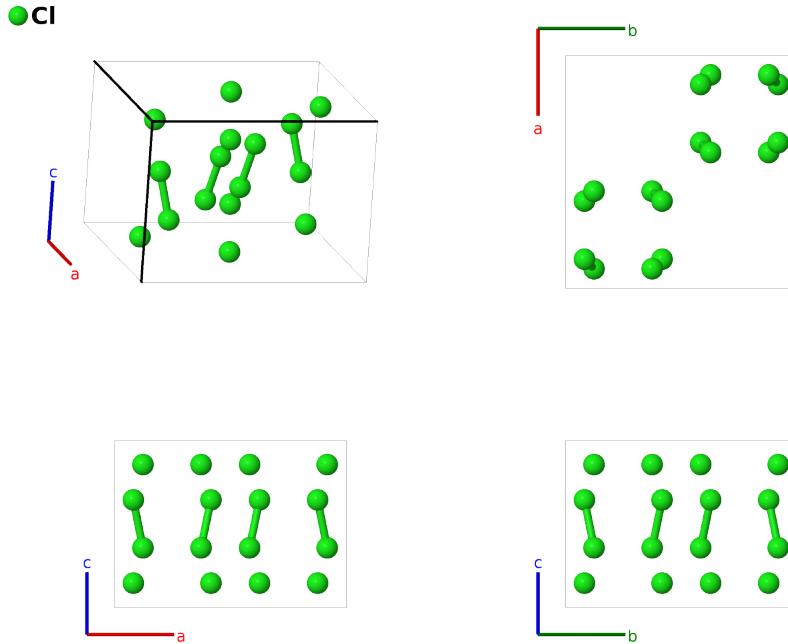
Cl (*A*18) Structure (*Obsolete*): A_tP16_138_j-001

This structure originally had the label A_tP16_138_j. Calls to that address will be redirected here.

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<https://aflow.org/p/ZBJR>

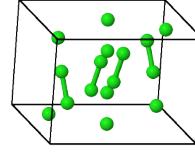
https://aflow.org/p/A_tP16_138_j-001



Prototype	Cl
AFLOW prototype label	A_tP16_138_j-001
Strukturbericht designation	A18
ICSD	22406
Pearson symbol	tP16
Space group number	138
Space group symbol	$P4_2/nm$
AFLOW prototype command	aflow --proto=A_tP16_138_j-001 --params=a, c/a, x1, y1, z1

- As given, this structure has a Cl-Cl bond distance of 1.82 Å, far too small for chlorine. The structure was eventually reanalyzed, and found to be similar to molecular iodine (A14). See (Donohue, 1982, p. 396) for details. We retain this structure for its historical interest. Note that all atoms are on the general sites of space group $P4_2/nm$ #138.

Simple Tetragonal primitive vectors



Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$a x_1 \hat{\mathbf{x}} + a y_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_2	$-\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_3	$-\left(y_1 - \frac{1}{2}\right) \mathbf{a}_1 + x_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$-a \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_4	$y_1 \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$a y_1 \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_5	$-x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$-a x_1 \hat{\mathbf{x}} + a \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_6	$\left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a y_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_7	$\left(y_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$a \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_8	$-y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$-a y_1 \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_9	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$-a x_1 \hat{\mathbf{x}} - a y_1 \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_{10}	$\left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_{11}	$\left(y_1 + \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$a \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_{12}	$-y_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$-a y_1 \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_{13}	$x_1 \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$a x_1 \hat{\mathbf{x}} - a \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_{14}	$-\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a y_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_{15}	$-\left(y_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$-a \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(16j)	Cl I
\mathbf{B}_{16}	$y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$a y_1 \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(16j)	Cl I

References

- [1] W. H. Keesom and K. W. Taconis, *On the crystal structure of chlorine*, Physica **3**, 237–242 (1936), doi:10.1016/S0031-8914(36)80226-2.

Found in

- [1] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).